



# Duquesne University Undergraduate Research Program

presents

## The 2002 Summer Research Symposium

sponsored by

The Bayer School of Natural  
and Environmental Sciences

*Keynote Address :*  
*Cyril Wecht, M.D., J.D.*  
*"Some of my Most  
Interesting Cases"*



Friday  
July 26, 2002  
9:00 a.m. - 4:00 p.m.  
Duquesne University  
Mellon Hall of Science, Pittsburgh, PA



## Plenary Session Schedule Pappert Hall Bayer Learning Center

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10:00 AM	Welcome	Dr. David Seybert, Dean, Bayer School of Natural and Environmental Sciences, Duquesne University
10:10 AM	Keynote Address	Dr. Cyril Wecht, M.D., J.D., Coroner of Allegheny County, <b>"Some of my most interesting cases"</b>
11:00 AM	Student Presentations	
	Michelle Sabo	<b>Isolation of the <i>Vgl</i> gene from the frog <i>Rana pipiens</i></b> Department of Biological Sciences, Duquesne University
	Shawn Badlani	<b>The Use of Matrix Metalloproteases (MMPs) to Digest Scar Tissue in Muscle</b> Pittsburgh Tissue Engineering Initiative Department of Orthopaedic Surgery, Children's Hospital and University of Pittsburgh, Musculoskeletal Research Center
	Heather MacPherson	<b>Crystalline Colloidal Array Photonic Crystals Glucose Sensors for Noninvasive Monitoring of Glucose in Tear Fluid</b> Department of Chemistry, University of Pittsburgh
11:45 AM	Short Break	
	Steve M. Ascencio	<b>3-D Technology in the Classroom</b> Department of Chemistry, University of Pittsburgh
	Dionne Leah Cozier	<b>Fenretinide and Dendritic cells</b> Department of Biochemistry and Chemistry, Duquesne University
	Martha Ottenberg	<b>Novel Assays of Biocompatibility of Ventricular Assist Devices implanted in Bovines</b> Chemical & Petroleum Engineering Department, University of Pittsburgh
	Amy Graveline	<b>The Effect of Silver Ions on Deep Wound Infections</b> Health Sciences Department Duquesne University Department of Electrical & Computer Engineering, Carnegie Mellon University
	Emily Belz	<b>Effects of Environmental Enrichment on Stress-Responsive Hormones in Laboratory Rats</b> Center for Neurosciences Research, Allegheny General Hospital
	Session Moderators	Dr. Partha Basu, Department of Chemistry and Biochemistry Dr. Daniel K. Donnelly, Center for Environmental Research & Education



## 2002 Summer Research Symposium Abstract Index

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### MOLECULAR DYNAMICS OF MOLECULAR HYDROGEN ADSORBED IN A C60 LATTICE

Ben Anderson, Dr. Karl Johnson, Xiongce Zhao

Chemical and Petroleum Department, University of Pittsburgh

It is known that hydrogen gas can adsorb into the octahedral sites of crystalline (fcc) C60. This has implications in the field of hydrogen storage, as in fuel cells. A molecular dynamics program has been developed to model the behavior of C60 and H2 at room temperature. The objective of this study is to compute the structural, energetic, and dynamic properties of this adsorbed hydrogen. Both species were modeled as Lennard-Jones spheres, and the cross interactions are calculated using Lorentz-Bethelot combining rules. The velocity Verlet algorithm was employed to solve the equations of motion. Velocity scaling, the Andersen thermostat, and Nosé-Hoover chains were all implemented as options for temperature control in constant-NVT ensembles. The equilibrium spacing within the face-centered cubic C60 lattice has been computed, as has the binding energy of hydrogen as a function of filling. The simulation results are compared with experimental results where possible.

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### Oral Presentation

#### 3-D TECHNOLOGY IN THE CLASSROOM

Steve M. Ascencio, John T. Johnson, Michelle L. Price, Dr. Joseph Grabowski, Dr. Kenneth Jordan, Christian Schafmeister  
Department of Chemistry, University of Pittsburgh

Students traditionally have difficulty with visualizing the three-dimensionality of chemical principles when described to them in traditional classrooms. Conventional teaching methods in chemistry such as the chalk board and molecular model kits are useful in portraying the true nature of molecules and molecular interactions, but are often insufficient to ensure complete student comprehension. Even "pseudo" 3-D programs (i.e., Chime, Rasmol) only simulate 3-D in two dimensions via changes in shading or rotation. It is now feasible, and the goal of this effort, to use modern technology to project computer generated three-dimensional images in large lecture halls. Our project's focus is to (1) implement user friendly hardware for 3-D projection in a 125-seat lecture hall; (2) develop software to increase faculty use of the 3-D system; and (3) develop teaching aids that take advantage of the hardware and software. Our experiences and progress to date will be discussed in this presentation.

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### DEVELOPMENT OF THE PHYSIO-FLOW: A NOVEL IN VITRO PRESSURE AND FLOW REGULATOR

Khashayar Attar-Toossi, Brian Wessel, Megan Rothney, Christian Sander, Stewart Lindquist, Dr. Sanjeev Shroff

Chemical and Petroleum Department, University of Pittsburgh

Studies in mechanobiology suggest there is an important distinction between the behavior of blood vessels in steady and pulsatile flow conditions. The steady and pulsatile aspects of pressure and flow are independent determinants of a number of vascular biological responses, the exact mechanisms of which are unknown. Unfortunately, current testing systems are inadequate--they cannot accurately generate physiologically relevant pulsatile waveforms. The main goal is to develop an in vitro flow loop wherein the user can independently and simultaneously specify pressure and flow waveforms through a given test specimen.

So far, a number of achievements have brought the PHYSIO-Flow closer to its ultimate goal. A mathematical model, based on a circuit analogue has been solved to serve as proof of principle. The model functions correctly for a number of tube stiffness values. It has been further adapted to consider the physical limitations of the pumps, such as response time and maximum force generation. The model also includes a number of physiological pressure and flow waveforms, which it can accurately emulate. A physical system where mean pressure and mean flow are fully managed by the computer in custom, closed loop control software has been implemented. A library of relevant physiological pressure and flow waveforms has been developed to test system performance.